P1 Wine

Huseyin Coskun/Ruben Garzon 15 Nov 2014

We will first read the Dataset obtained from UCI ML repository https://archive.ics.uci.edu/ml/datasets/Wine

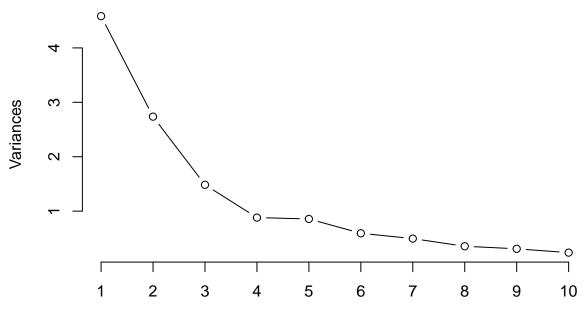
```
wine <- read.csv("../Datasets/Wine/wine.data", header=FALSE)
colnames(wine) <- c("class", "Alcohol", "Malic Acid", "Ash", "Alcalinity of Ash", "Magnesium", "Total Phenols</pre>
```

We can plot the data with PCA to explore the distribution of classes (UNIFINISHED)

plot(wine.pca, type = "1")

```
# log transform
log.wine <- log(wine[, 2:14])
# apply PCA - scale. = TRUE is highly
# advisable, but default is FALSE.
wine.pca <- prcomp(log.wine,
                 center = TRUE,
                 scale. = TRUE)
summary(wine.pca)
## Importance of components:
                                  PC2
                                        PC3
                                               PC4
                                                      PC5
                                                              PC6
                                                                     PC7
##
                            PC1
## Standard deviation
                          2.141 1.654 1.218 0.9386 0.9254 0.7699 0.7036
## Proportion of Variance 0.353 0.210 0.114 0.0678 0.0659 0.0456 0.0381
## Cumulative Proportion 0.353 0.563 0.677 0.7449 0.8108 0.8564 0.8945
##
                             PC8
                                    PC9
                                          PC10
                                                 PC11
                                                         PC12
## Standard deviation
                          0.5953 0.5544 0.4872 0.4500 0.3886 0.34524
## Proportion of Variance 0.0273 0.0236 0.0183 0.0156 0.0116 0.00917
## Cumulative Proportion 0.9217 0.9454 0.9636 0.9792 0.9908 1.00000
```

wine.pca



We will first create the training and test with alpha = 0.6 (same value used in the paper)

```
library(caret)
```

```
## Loading required package: lattice
## Loading required package: ggplot2
inTrain <- createDataPartition(wine$class, p=0.6, list=FALSE)
trainingSet <- wine[inTrain,]
testSet <- wine[-inTrain,]</pre>
```

We would need to scale the variables, but svm seems to do this for us, so at the moment we will not do this. We apply SVM for prototype selection. We will choose the support vectors as prototypes, although some improvement could be done.

```
library(e1071)
library(caret)
svmfit=svm(class~., data=trainingSet, kernel="linear", cost=10,scale=FALSE)
prototypes<-trainingSet[svmfit$index,]</pre>
```

We now compute the Disimilarity matrix using Euclidean distance The method dist is returning a vector with the lower triangle of the computed distances. This is not easy because we need to concatenate samples matrix + prototype matrix and then select only the elements of the resulting vector from applying dist that we are interested in.

```
distances <- dist(rbind(trainingSet[,-1],prototypes[,-1]),method="euclidean")
elements <- nrow(trainingSet)*nrow(prototypes)
lowindex <- nrow(trainingSet)-1
upindex <- lowindex + elements -1
relevantDistances <- distances[lowindex:upindex]
dissimilarities <- matrix(relevantDistances,nrow=nrow(trainingSet),ncol=nrow(prototypes))</pre>
```

Now we should apply QDA to the dissimilarity training space Question, in the paper they compare by number of prototypes, should we also do all this tests with different number of prototypes?